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Pulse frequency effect on neutron damage in -Iron: A KMC analysis

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The pulsed nature of the irradiation and the high neutron dose are the critical factors in an Inertial Fusion Energy reactor (IFE). The damage that structural materials suffer under these extremes conditions require a careful study and assessment. The goal of our work is to simulate, trough the multiscale modelling approach, the damage accumulation in α-Fe under conditions relevant to a IFE Reactor. We discuss how the pulse frequency, 1 Hz, 10 Hz, and the dose rate of 10__ and 10__ dpa/s affect the damage production and accumulation. Results of the damage that this demanding environment can produce on a protected first structural exposed to 150 keV average recoil ion will be presented. A further comparison it has been made with the damage produced by a continuous irradiation at similar average dose.

Introduction

Some designs of future fusion reactors consider the possibility of utilizing steels as the structural wall material [1]. These materials are put under very demanding conditions in fusion reactors. An accumulation of more than 30 dpa can be expected during their lifetime in the reactor. Specifically in Inertial Fusion Reactors there is a key additional factors that can influence the formation and evolution of defects and therefore the change of mechanical properties of the materials; that is the pulsed nature of the neutron, x-rays and charged particles irradiation. It is therefore necessary a complete study of the evolution of the macroscopic and microscopic magnitudes under such differential characteristic in order of being able to estimate the response of the above mentioned steel. This result, untill to day, can be only achieved trough multiscale modeling (computational simulation processes). An adequate neutron source able to reproduce the characteristics of such pulse irradiation does not actually exist, but some proposals have appeared in last few years [2]. We analyze in this work the microscopic response of pure α-Iron (as the main steel component) under two different dose rates, with two different pulse rate frequencies, and for two temperatures, with the intention of reproducing the damage suffered by a structural wall receiving mainly irradiation of highest energy fusion neutrons (14 MeV). A preliminary presentation of the computational modeling is given. It is also necessary to justify the dose rates and frequency conditions adopted in this work, in comparison with previous computational analysis [3] using with similar methodologies.

Simulation model

The MonteCarlo method applied to transport calculations is a stochastic algorithm that allows the knowledge of life behavior of the interested population through a well-defined sequence of events, which happens with a known probability distribution. MC is, because of this characteristic, a suitable and very useful tool to study the evolution of the microstructure of an irradiated material, extended to long times. The simulations herein presented have been performed with a Kinetic Monte Carlo program (KMC), in which the crystal structure is not taken into account. The program employed is BIGMAC developed at the Lawrence Livermore National Laboratory (LLNL) originally thought to describe Boron diffusion in Silicon and lately utilized to model the development of the defects complex produced by cascades in various metals [4], [5]. BIGMAC is an efficient KMC program in which a "population" of defects is followed in its evolution.
As mentioned before, in order to be able to perform our KMC simulations, a well-defined series of input data is needed. We need to know what, the various species are that constitute the population, what the characteristics of each species are, and the reactions that might occur between each one of them. In our simulation we have considered punctual defects (vacancy and interstitial), defects clusters, considering each size as a different object, and impurities. Impurities have been considered immobile, transparent to vacancies and able to react only with interstitials with a binding energy of 1.0 eV. Seven possible events have been considered:

1) Diffusion, 2) Clustering of defects of the same type, 3) Dissociation of a particle from a cluster, 4) Annihilation of defect of opposite type, 5) Annihilation of defects in Sink, 6) Trapping, 7) New Cascade

Each object in the simulation box has an associated set of probabilities corresponding to the undergoing events. All simulations have been conducted in a 300 nm cubical box. The parameters we have considered are the dose rate (0.1 - 0.01 dpa/s), the pulse frequency (1 - 10 Hz) and the temperature (300 – 600 K).

Dose Rates in Inertial Fusion Reactors.

The nature of energy generation by Inertial Fusion [6] is intrinsically pulsed. The microexplosion produced after the high-density compression of a more or less complex DT target liberates a high intensity pulse of neutrons (75 %), X-rays (20 %) and charged particles (5%). That fraction is very much dependent of the class of target considered (direct or indirect [hohlraum] targets). Assuming an energy gain of ≈ 100-200 for ignition conditions with a driver-energy on target of ≈ 10-5 MJ, it could be possible to obtain ≈ 1000 MJ per pulse. If the repetition rate of the driver is 5-10 Hz (5-10 times per second) then the power in the system reaches ≈ 5-10 GW, well in the range needed for driver efficiencies of 10 % in laser and efficient systems of fusion. It is certainly clear that the four parameters (driver energy, target energy gain, driver frequency, power requested) are interconnected and technological achievements in some of their conditions influence the request in the others. Assuming a fixed goal of 1 GW net considering the driver efficiency and ignition from 5 MJ there could be solutions for high energy per pulse which allow to decrease the frequency, or less demanding energy gains with higher frequency of the high energy driver.

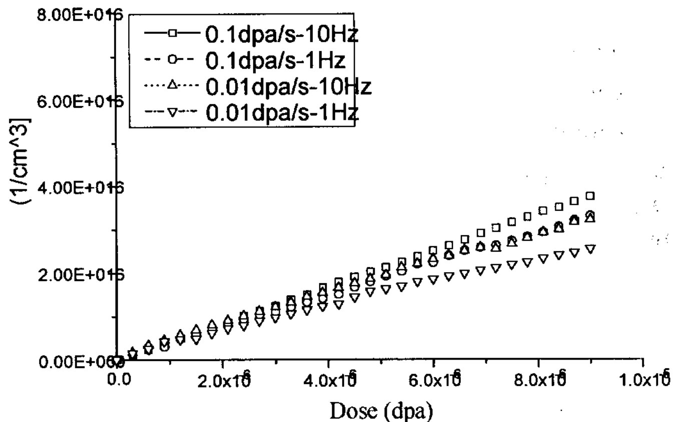

Fig. 1 Vacancy cluster concentration

The interest for these calculations (in order to be most realistic) is to estimate the dose rate received by the structural material. A systematic study of such conditions can be found in Perlado [7], and we present now the relevant numbers for this study. The first magnitude is the neutron intensity from the target that is in the range of 10^{21} n.s^{-1} on average for output of 600 MJ and 3 Hz. The second parameter in the emission is the energy spectrum that is modified depending on the constituent's elements of the target and the degree of compression; it has been estimated in average in 10-12 MeV. The third parameter is the time in which the microexplosion is produced which is in the range of hundreds of picoseconds. Using these emission parameters it is now possible to transport the neutron through the engineering concept to obtain the irradiation flux and energy spectrum in the material of our interest. The key conditions to obtain such results are the radius of the chamber of the reactor and the dimensions and composition of the blanket with the functions of energy transmission and breeding of tritium. We use here the results from calculations performed considering a radius of 7 m and an effective protection of 66 cm of $Li_{17}Pb_{83}$ that was considered the coolant for some concepts. The results are given on dpa_{NRT} on Fe and the production of gaseous impurities (He). The Table 1 gives the peak results for different conditions of protection and no-protection of the chamber. The other key parameter is the time duration of such intense deposition on the Fe wall that is of $\approx 1\mu$s assuming such irradiation after transport through the blanket. In a realistic case the peak (0.01 -0.02 dpa/s) is attained 130 ns after the neutron burst corresponding with the 14 MeV neutrons. A new peak is observed at 170 ns corresponding to the more energetic neutrons moderated on the blanket. A large difference is observed for bare walls of Fe where the displacement damage is large up to 25 dpa/s but produced in the time of flight of neutrons (dependence of radius) that can be estimated in the range of 100 ns in total duration. Then we decide to consider conditions for inertial fusion in the range of 0.01 – 0.1 dpa/s with duration of pulse in the material of 1μs.

The following magnitude necessary for calculations is the Primary Knock-on Atom (PKA) energy spectra. Different spectra have been computed for different neutron irradiation using the SPECTER code [8], and they are represented in Perlado [9]. It has been reported average neutron energies of 2-4 MeV in unprotected walls (due to slowing-down of backscattered neutrons) with recoils in average of 30-40 keV, and neutron energies of hundreds of keV for protected walls with recoils in the range of some few keV. In our calculations here we have been using the worst case; recoils of 150 keV in average have been considered as starting the cascades. This is certainly a key parameter when comparing these results with those reported previously with a spectral tailoring. That value in the PKA energy is coherent with almost monoenergetic neutrons in the range of 14 MeV. Previous reported results [10] indicate that for 14 MeV neutrons almost 45% of recoils have energies larger than 200 keV producing 75 % of displacement, and 60 % of recoils have energies larger than 100 keV producing 90% of displacement. For slowed-down neutrons existing in the first wall, the recoils with energies > 100 keV is only of 11 % producing 70 % of displacements. With these assumptions we are certainly estimating an upper bound of results considering that 14 MeV neutrons are irradiating Fe in 1μs not following the decrease in dose rate and energy of neutrons as indicated in transport calculations [7].

Table 1.- Dose Rates and Gaseous production rates in pulsed IFE chamber protections

Structural Material	HT9 (assumed Fe)	HT9 (assumed Fe)	HT9 (assumed Fe)	HT9 (assumed Fe)
Neutron Source	Spectral <10 MeV>	Spectral <10 MeV>	Spectral <10 MeV>	Monoenergetic 14 MeV
Effective Thickness (Li_{17} Pb_{83})	66 cm	0 (Bare Wall)	133 cm	66 cm
Peak (dpa/s)	0.013	25	0.0014	0.018
Peak (appm He/s)	0.17	220	0.00012	0.24

Results

The starting point of the simulation is the primary damage state, represented by spatially distributed defects, obtained as result of displacement cascade. All simulations have been conducted in a 300 nm cubic box. The energy of the PKA introduced in each pulse, as extensively explained in the previous section, is of 150 keV. We utilized some cascades produced by the authors and mainly an already existent data base [11]. The maximum energy available in the cascades data base is of 50 keV that means that we need to build our recoil ion as a composition of less energetic ions. The composition of various ions has been done estimating the distribution of subcascades generated by the 150 keV ion with the program TRIM [12] which provide us the necessary information concerning the energy and spatial distribution of the produced recoils. We simulated pulse repetition rate of 1 and 10 Hz at 300 K for the two dose rate considered and we also simulated pulsed irradiation at 600 K with 0.1 dpa/s and with a repetition rate of ten times per second (10 Hz). The high energy of the recoil and its numerous associated defects, that in each pulse were introduced in the box, are the responsible for slowing down the simulation and make computational time largely grow, together with the low migration energy of the interstitials cluster. We have been able to perform 1000 pulse with the dose rate of 0.01 dpa/s and 100 pulses with 0.1 dpa/s dose rate which make the reached dose of the order of 10^{-5} dpa.

Figure 1 and Figure 2 show vacancy cluster concentration and trapped interstitial concentration.From these plots it can be argued that, the bigger is the dose rate and the higher is the frequency, more vacancy clusters appear to be in the box. This can be explained trough the simple consideration that under these conditions we are introducing more defects and giving them less time to anneal out. We can also explain the fact that the two "intermediate" curves follows the same values. In fact a lower level of dose rate is compensated by an higher frequency and a higher level of dose is smoothed by a lower frequency. Vacancy cluster average size, Figure 3, has a clear dependence with the frequency. Lower is the frequency, higher is the average size, the explanation of this phenomenon is that the growth of vacancy cluster is time among pulses dependent.

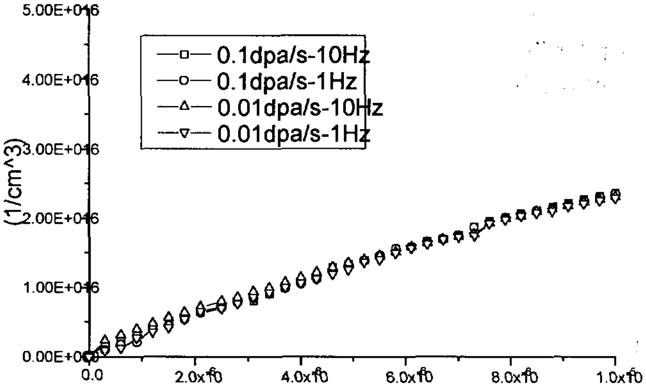

Fig. 2 Trapped interstitials concentration vs Dose

Short time among pulses does not allow vacancy to migrate and to increase the size of the existing vacancy clusters. Whereas interstitial trapping is not influenced by the pulse rate. This effect can be understood due to the high velocity of migration of the interstitial cluster. That lead to the consequence that any events involving interstitials is already over before the arrival of another pulse, Figure 2. In fact no acceptable difference can be extrapolate among the curves. No sessile interstitial clustering has been recorded in any of the simulations. Continuous irradiation show the same effect of pulsed radiation with 1Hz frequency as shown in Figure 4, which is essentially consistent with previous work [3].

At 600 K only thirty pulses have been accumulated and no significant conclusion can be attained due to the very low dose level reached. Fig.3 The results of this simulation although in contrast with previous work conducted with kinetic rate theory [13], which previewed a higher concentration of loops in the pulsed system show a good agreement with other works [3] in which the cluster interstitial migration has been kept in count.

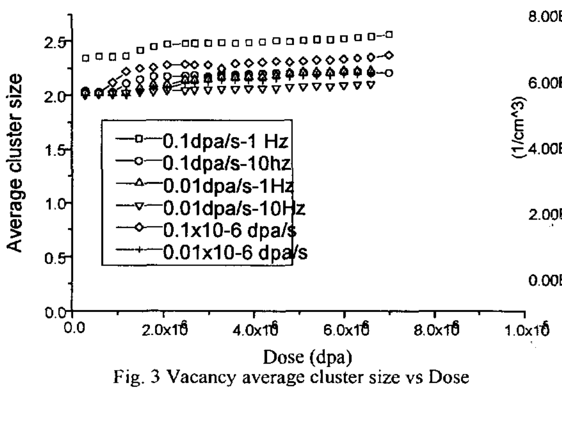

Fig. 3 Vacancy average cluster size vs Dose

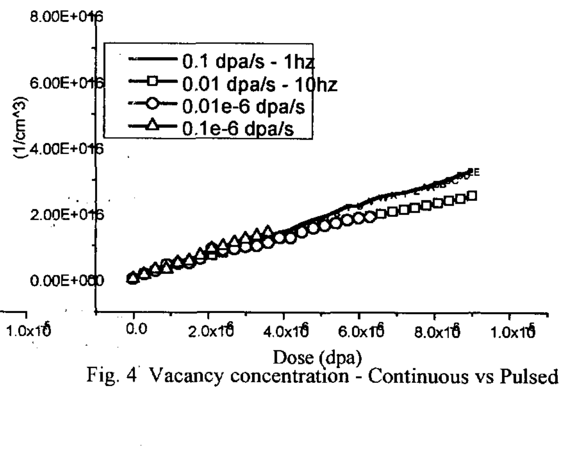

Fig. 4 Vacancy concentration - Continuous vs Pulsed

Conclusion

The results show clearly that the velocity of migration of vacancies and interstitials play an important role in defects accumulation. In fact the variable that control vacancy cluster accumulation and cluster average size is the frequency. We conclude that the more time have defects to migrate the bigger is the size of the cluster, and the higher is the frequency the bigger is cluster accumulation. No difference has been noticed between pulsed and continuous for the same integrated dose.

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